Molecular modeling within zeolite catalysis : The Methanol-to-Olefin process as a case study

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Zeolites are amongst the most widely investigated and topical of inorganic materials. They are widely used in industry for a plethora of applications. Within this contribution we specifically highlight meticulous design of zeolites for catalysis. The Methanol to Olefins reaction is chosen as a case study to highlight the subtle interplay between various factors leading to catalysts with longer lifetime and/or better selectivity towards the desired olefins. Molecular modeling in close synergy with experimentalists is crucial in understanding the function and nature of the active site. However modeling efforts need to account for realistic working conditions such as the true nature of the feedstock, framework flexibility, temperature and pressure effects, competitive pathways,… Our approach consists in simulating complex chemical transformations in nanoporous materials using first principle molecular dynamics methods at real operating conditions, capturing the full complexity of the free energy surface. The subtle interplay between various factors enable to enhance the product selectivity or to suppress or enhance the aromatic cycle leading to more or less propene formation. Within this contribution, we will highlight the impact of zeolite acidity, feed composition, temperature, and post-synthetic modification to enhance the olefin selectivity. Recently it was shown that post-synthetic incorporation of alkaline earth metals in H-ZSM-5 may also enhance olefin selectivity. It is an example of how meticulously tuning the active site may impact the lifetime of the catalyst and product selectivity. Herein we give molecular level understanding in the nature of the active sites. Throughout the talk we show to importance of modeling techniques that account for realistic working conditions. The approach followed here may greatly impact catalysis science and reveal insights that were undiscovered so far.